Superdense Crystal Packings of Ellipsoids

Aleksandar Donev[1,2], Frank H. Stillinger[4], P. M. Chaikin[2,3], and Salvatore Torquato[1,2,4*]

[1]*Program in Applied and Computational Mathematics,*

Princeton University, Princeton, NJ, 08544

[2]*Princeton Materials Institute, Princeton, NJ, 08544*

[3]*Department of Physics, Princeton University, Princeton, NJ, 08544 and*

[4]*Department of Chemistry, Princeton University, Princeton, NJ, 08544*

Abstract

Particle packing problems have fascinated people since the dawn of civilization, and continue to intrigue mathematicians and scientists. Resurgent interest has been spurred by the recent proof of Kepler's conjecture: the face-centered cubic lattice provides the densest packing of equal spheres with a packing fraction $\varphi \approx 0.7405$ [1]. Here we report on the densest known packings of congruent ellipsoids. The family of new packings are crystal (periodic) arrangements of nearly spherically-shaped ellipsoids, and always surpass the densest lattice packing. A remarkable maximum density of $\varphi \approx 0.7707$ is achieved for both prolate and oblate ellipsoids with aspect ratios of $\sqrt{3}$ and $1/\sqrt{3}$, respectively, and each ellipsoid has 14 touching neighbors. Present results do not exclude the possibility that even denser crystal packings of ellipsoids could be found, and that a corresponding Kepler-like conjecture could be formulated for ellipsoids.

BACKGROUND

Dense packings of nonoverlapping particles have been employed to understand the structure of a variety of many-particle systems, including glasses [2], crystals [3], heterogeneous materials [4], and granular media [5]. The famous Kepler conjecture postulates that the densest packing of spheres in three-dimensional Euclidean space has a packing fraction (density) $\varphi = \pi/\sqrt{18} \approx 0.7405$, as realized by stacking variants of the face-centered cubic (FCC) lattice packing. It is only recently that this conjecture has been proved [1, 6]. Very little is known about the most efficient packings of convex congruent particles that do not tile three-dimensional space [7, 8]. The only other known optimal three-dimensional result involves infinitely long circular cylindrical particles: the maximal packing density $\phi_{\max} = \pi/\sqrt{12}$ is attained by arranging the cylinders in parallel in the triangular lattice arrangement [9]. Of particular interest are dense packings of congruent ellipsoids (an affine deformation of a sphere) with semi-axes a, b and c or, equivalently, with aspect ratios $\alpha = b/a$ and $\beta = c/a$.

In two dimensions, it can easily be shown that the densest packing of congruent ellipses has the same density as the densest packing of circles, $\varphi = \pi/\sqrt{12} \approx 0.9069$ [10, 11]. This maximal density is realized by an affine (linear) transformation of the triangular lattice of circles. Such a transformation leaves the density unchanged. In three dimensions attempts at increasing the packing density yield some interesting structures, at least for needle-like ellipsoids. By inserting very elongated ellipsoids into cylindrical void channels passing through the ellipsoidal analogs of the densest ordered sphere packings (an affinely deformed face centered cubic or hexagonal close packed lattice), congruent ellipsoid packings have been constructed whose density exceeds 0.7405 and approaches 0.7585 in the limit of infinitely thin prolate spheroids (ellipsoids of revolution), i.e., when $\beta = 1$ and $\alpha \to \infty$ [9, 12].

However, there appears to be a widespread belief that for nearly spherical ellipsoids the highest packing fraction is realized by an affine transformation (stretch by α and β along two perpendicular axes) of the densest sphere packing, preserving the density at 0.7405. Mathematicians have often focused on *lattice packings*, where a single particle is replicated periodically on a lattice to obtain a crystal packing. For ellipsoids, a lattice packing is just an affine transformation of a sphere packing, and therefore a theorem due to Gauss [7, 8] enables us to conclude that the densest lattice ellipsoid packing has $\varphi \approx 0.7405$. The next level of generality involves nonlattice periodic packings (lattice packings with a multiparticle basis),

where a unit cell consisting of several ellipsoids with at least two *inequivalent* orientations is periodically replicated on a lattice to fill Euclidean space. We will refer to these as *crystal packings*.

We present here a family of crystal packings of ellipsoids that are denser than the best lattice packing for a wide range of aspect ratios in the vicinity of the sphere point $\alpha = \beta = 1$, and for certain aspect ratios yields the densest known ellipsoid packings with $\phi \approx 0.7707$.

THE DISCOVERY

We recently developed a molecular dynamics technique for generating dense random packings of hard ellipsoids [13]. The simulation technique generalizes the Lubachevsky-Stillinger (LS) sphere-packing algorithm [14] to the case of ellipsoids. Initially, small ellipsoids are randomly distributed and randomly oriented in a box with periodic boundary conditions and without any overlap. The ellipsoids are given velocities and their motion followed as they collide elastically and also expand uniformly, while the unit cell deforms to better accommodate the packing. After some time, a jammed state with a diverging collision rate is reached and the density reaches a maximal value.

Using this technique, we generated nonequilibrium random close packings of ellipsoids and observed that for certain aspect ratios (close to $\alpha \approx 1.25$, $\beta \approx 0.8$) the random packings had a density as high as 0.735, surprisingly close to what we believed was the densest ordered packing (stretched FCC lattice) [15]. This brought into question what the maximal density really was for those aspect ratios. Extensive experience with spheres has shown that for reasonably large packings, sufficiently slowing down the growth of the density, so that the hard-particle system remains close to the equilibrium solid branch of the equation of state, leads to packings near the FCC lattice [16, 17]. This however requires impractically long simulation times for large ellipsoid packings. By running the simulation for very small unit cells, from 4 to 16 particles per unit cell, we were able to identify crystal packings significantly denser than the FCC lattice, and subsequent analytical calculations suggested by the simulation results led us to discover ellipsoid packings with a remarkably high density of $\phi \approx 0.7707$. This result implies a lower bound on the maximal density of any packing of congruent ellipsoids, namely, $\varphi_{\max} \geq 0.7707$.

SUPERDENSE LAMINATED PACKINGS OF ELLIPSOIDS

We now describe the construction of a family of superdense crystal packings of ellipsoids. We start from the FCC lattice, viewed as a laminate of face-centered planar layers of spheres, as illustrated in Fig. 1a. We similarly construct layers from the ellipsoids by orienting the c semiaxis perpendicular to the layer, while orienting the a and b axes along the axes of the face-centered square lattice defining the layer, as shown in Fig. 1b. In this process, we maintain the aspect ratio of the squares of side L of the face-centered square lattice defining the layer, i.e., we maintain

$$L = \frac{4\alpha}{\sqrt{1 + \alpha^2}}, \tag{1}$$

which enables us to rotate the next layer by $\pi/2$ and fit it exactly in the holes formed by the first layer. This two-layer lamination is then continued *ad infinitum* to fill all space. This can be viewed as a family of crystal packings with a unit cell containing two ellipsoids.

We can calculate the minimal distance h between two successive layers (that preserves impenetrability) from the condition that each ellipsoid touches four other ellipsoids in each of the layers above and below it. This gives a simple system of equations (two quadratic equations and one quartic equation), the solution of which determines the density to be

$$\phi = \frac{16\pi\alpha\beta}{3hL^2}. \tag{2}$$

Notice that the axis perpendicular to the layers can be scaled arbitrarily, without changing the density. We can therefore just consider spheroids with $\beta = 1$. The density of this crystal packing as a function of the aspect ratio α is shown in Fig. 2a, and is higher than the density of the FCC sphere packing for a wide range of aspect ratios around the sphere point $\alpha = \beta = 1$, symmetrical with respect to the inversion of α between prolate and oblate ellipsoids (we consider the prolate case in the equations in this section). Two sharp maxima with density of about 0.770732 are observed when the ellipsoids in the face-centered layers touch six rather than four inplane neighbors, as shown in Fig. 2b, i.e., when $L = 2\alpha$, which gives $\alpha = \sqrt{3}$ for the prolate and $\alpha = 1/\sqrt{3}$ for the oblate case. These two densest-known packings of ellipsoids are illustrated in the insets in Fig. 2a, and in these special packings each ellipsoid touches exactly 14 neighboring ellipsoids (compare this to 12 for the FCC lattice).

THE FUTURE

There is nothing to suggest that the crystal packing we have presented here is indeed the densest for any aspect ratio other than the trivial case of spheres. Many other possibilities exist for laminated packings with alternating orientations between layers, and one such example is shown in Fig. 3. More generally, we believe it is important to identify the densest periodic packings of ellipsoids with small numbers of ellipsoids per unit cell. This may be done using modern global optimization techniques, as has been done for various sphere and disk packing problems. However, this is a challenging project due to the complexity of the nonlinear impenetrability constraints between ellipsoids. In particular, the case of slightly aspherical ellipsoids is very interesting, as the best packing will be a perturbation of the FCC lattice with a broken symmetry, and should thus be easier to identify. In Fig. 2b we see that the density of our crystal packing increases smoothly as asphericity is introduced, unlike for random packings, where a cusp-like increase is observed near $\alpha = 1$ [15]. Is there a crystal packing which leads to a sharp increase in density for slightly aspherical ellipsoids? Further multidisciplinary investigations are needed to answer this and related questions. The results of such investigations could be used to formulate a Kepler-like conjecture for ellipsoids.

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FIGURES

Figure 1: *Part a (top):* The face-centered cubic packing of spheres, viewed as a laminate of face-centered layers (bottom layer is colored purple and the top layer yellow). *Part b (bottom):* A nonlattice layered packing of ellipsoids based on the FCC packing of spheres, but with a higher packing fraction.

Figure 2: *Part a (top):* The density of the laminate crystal packing of ellipsoids as a function of the aspect ratio α ($\beta = 1$). The point $\alpha = 1$ corresponding to the FCC lattice sphere packing is shown, along with the two sharp maxima in the density for prolate ellipsoids with $\alpha = \sqrt{3}$ and oblate ellipsoids with $\alpha = 1/\sqrt{3}$, as illustrated in the insets. *Part b (bottom):* The layers of the densest known packing of ellipsoids, as illustrated in part a. The layers can be viewed as either face-centered or triangular.

Figure 3: Another computer-generated layered packing of prolate ellipsoids ($\alpha = \sqrt{3}$) with a zig-zag-like variation in the orientations of the ellipsoids in adjacent layers. This packing is slightly denser than the FCC lattice ($\varphi = 0.7411$), but we did not attempt to find the optimal configuration.
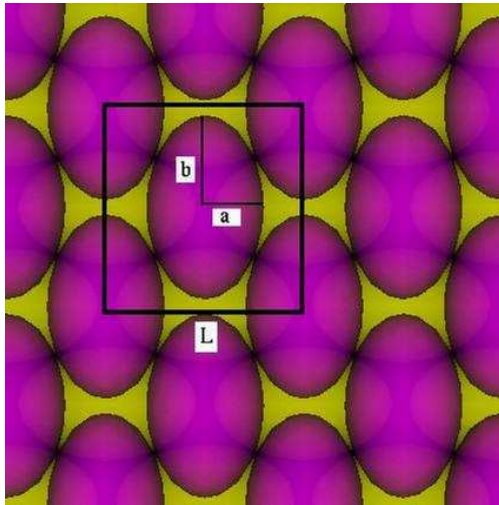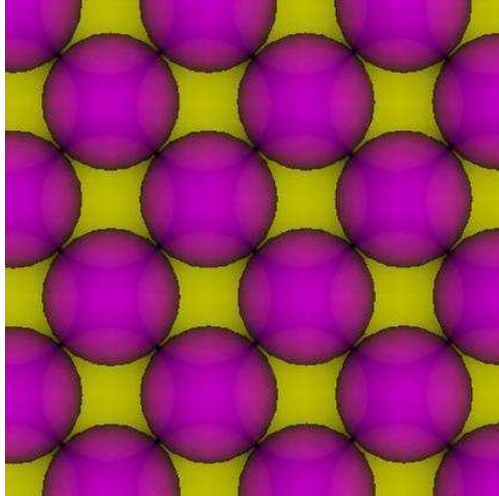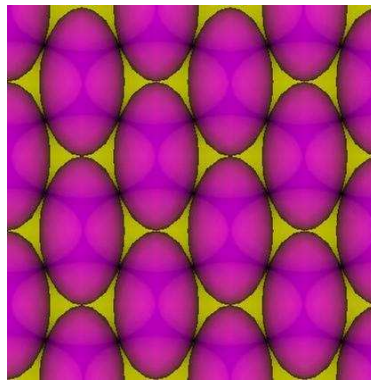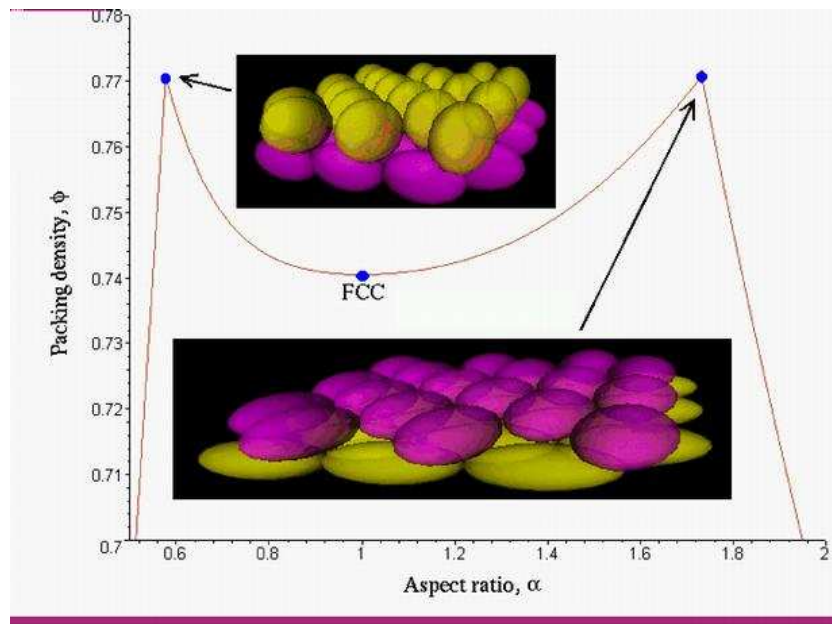
Figure 1: *Donev et al.*

Figure 2: *Donev et al.*

Figure 3: *Donev et al.*